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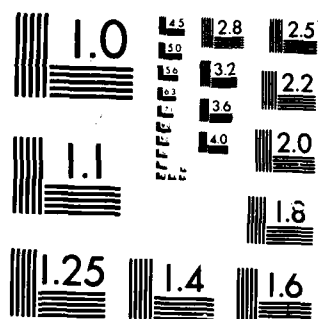
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A FUNDAMENTAL MATHEMATICAL THEORY FOR
THERMAL EXPLOSIONS IN RIGID SOLIDS AND IN GASES

AD-A164 692

Final Report
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J. Bebernes and D. R. Kassoy

January 31, 1986

U.S. Army Research Office

Contract DAAG 29-82-K-0069

University of Colorado, Boulder, CO 80309

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| 20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This research project has emphasized the formulation of rational mathematical models for transient and steady combustion processes. In particular thermal explosions, shock wave initiation and high speed combustion waves have been examined. In each case the describing mathematical system is analyzed using both formal and constructive techniques. The former are employed to consider issues of existence and uniqueness, solution bounds and general trajectory properties. Constructive solution development is based on a combination of | | |

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asymptotic and numerical methods. This hybrid approach to the study of combustion problems has permitted us to develop both a rigorous and quantitative understanding of complex, initial-boundary value problems. This report contains a summary description of each of the 20 papers contributed by the research group.

*Report to the
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I. Introduction

The initiation of a combustion process involves a myriad of complex physical phenomena which are fascinating to observe and challenging to describe in quantitative terms. In general one is concerned with the time history of a spatially varying process occurring in a deformable material in which there is a strong interaction between chemical heat release, diffusive effects associated with transport properties, bulk material motion as well as several types of propagating wave phenomena. Mathematical models capable of describing these combustion systems incorporate not only familiar reaction-diffusion effects associated with rigid materials but those arising from material compressibility as well. In the case of a combustible gas, the complete reactive Navier-Stokes equations are required to describe the phenomena involved.

During this 3 year research effort, the following topics have been considered: (1) thermal explosion processes in rigid combustible materials and in reactive gases; (2) steady state combustion waves with significant input Mach numbers; and (3) the generation of acoustic and shock waves by deposition of energy in a gas. Progress in each of the three areas is summarized below. More information descriptions of the significant results are described in greater detail in section II.

The major accomplishments of our thermal explosion work have been

- a) The development of constructive mathematical methods, based on asymptotic analysis, for handling complex chemical kinetics.
- b) The rational modeling of the induction period of a confined reaction in a gas, including the interaction between distributed energy addition and self-induced fluid motion including acoustic wave generation.

- c) A complete, rigorous mathematical description of the temperature for the induction period model and precise bounds on the thermal runaway time.
- d) Significant progress in describing rigorously how the hot spot solution profile develops in a neighborhood of the blow-up singularity.
- e) The development of formal mathematical methods for handling the complete one-dimensional model for a heat conductive, viscous, reactive gas bounded by two infinite parallel plates.

For combustion waves our work has shown that:

- a) transport properties can be ignored when considering the detailed dynamics of a high speed deflagration.
- b) the ignition process in a high speed deflagration resembles a convecting thermal explosion.
- c) the interaction of distributed heat addition and compressibility effects control the dynamics of the rapid phase of the high speed deflagration.
- d) the mathematical methods developed for thermal explosion problems are applicable to high speed combustion wave problems.
- e) the classical mathematical model of a doubly infinite flame is embedded in burner-attached flame theory for the limit of vanishingly small conductive heat transfer to the burner.

The study of gasdynamics wave generation shows that

- a) a quantitative source theory can be developed for wave generation which provides a precise relationship between wave amplitude and power addition at the boundary and/or power density in the heated layer.

- b) direct initiation of a strong shock requires an initial power pulse time close to the intermolecular collision value and a sustained heating rate of 1MW/m^2 over a longer period.
- c) observations of power requirements for direct initiation of detonation waves can be explained with the conceptual ideas developed for the generation of a shock wave in an inert gas.
- d) detonation wave initiation can be studied using concepts developed for shock wave generation problems.

II. Research Activities: A Summary

During the 3-year lifetime of the research project described in this Final Report the participants published 20 articles in peer-judged journals covering the fields of combustion science and applied mathematics. In addition a total of about 50 invited and contributed technical presentations were given in colloquia, seminars, short courses and technical meetings in Europe, Japan as well as the U.S.

Partly as a result of scientific accomplishments arising from ARO-supported work, J. Bebernes and D. R. Kassoy received the following fellowships, grants and recognition.

J. Bebernes

1. Invited talk, NSF-CBMS Conference on Combustion Theory, CSU, Fort Collins, June, 1982.
2. Invited participant, NATO Summer Conference on Partial Differential Equations, Oxford, England, August, 1982.
3. Mathematical Sciences Research Equipment Grant, NSF, \$115,000.
4. Invited talk, AMS Regional Meeting, University of Utah, Salt Lake City, April, 1983.

5. Invited talk, Oberwolfach, W. Germany, May, 1984.
6. Invited talk, SISA, Trieste, Italy, May, 1984.
7. Guest Lecturer, IX Scuola Estiva di Fisica Matematica. Presented 15 hour lectures on Mathematical Problems in Combustion Theory, Ravello, Italy, September, 1984.
8. "Mathematics of Thermal Explosions in Confined Reactive Gases", NATO Collaborative Research Grant Program, 12-17-84 to 1-31-86.

D. R. Kassoy

1. Senior Visiting Fellow of the Science and Engineering Research Council, United Kingdom, 1982-83.
2. Fulbright Research Grant to the Netherlands, 1983.
3. Faculty Fellowship, University of Colorado, 1982-83.
4. "Thermal explosions in confined reactive gas mixtures", U.S.-U.K. Cooperative Research Program. National Science Foundation, 9/1/83-2/28/87.
5. Scientific Computing Research Equipment, DOD Instrumentation Grant, \$120,000, 1985.
6. Fellowship from the Japan Society for the Promotion of Science, Nagoya University, June, 1985.
7. Invited article in Annual Reviews of Fluid Mechanics, "Mathematical modelling for planar, steady, subsonic combustion wave", *17*, 267-287 (1985).

Each of the papers published or submitted during the 3-year contract period are summarized briefly below. Several were initiated during an earlier contract period but were completed only during the period of the current contract.

D. R. Kassoy, "A note on asymptotic methods for jump phenomena", SIAM J. Appl. Math. **42**, 926-932, (1982).

Matched asymptotic expansion methods are employed to find a solution for

$$y' = y^2(1-y), \quad y(0) = \epsilon; \quad t \geq 0$$

in the limit $\epsilon \rightarrow 0$. In the first of three distinct regions $y = O(\epsilon)$ and grows, becoming singular when $t \rightarrow \epsilon^{-1}$. In a subsequent thinner transition zone where $y = O(\ln^{-1}(1/\epsilon))$, a nonuniformity occurs when $t \rightarrow t^*\epsilon^{-1} + \ln(\epsilon^{-1}-1)$. Finally an $O(1)$ jump in y occurs in a layer of $t = O(1)$. The results are compared with those found by Reiss [SIAM J. Appl. Math. **39**, 440-455 (1980)] who employed an approximate solution method. It is demonstrated that Reiss' results correspond to limited portions of the more precise solutions. The $O(1)$ -change in y near the jump location t^* is shown to be described quite accurately by the matched asymptotic solution when $\epsilon = 0.02$ and only very approximately by Reiss' method.

J. Bebernes and R. Ely, "Existence and invariance for parabolic functional equations", Nonlinear Anal. Theory, Methods, and Applications, **7** (1983), 1225-1236.

The temperature perturbation solution $\theta(x,t)$ of the induction period model for a reactive gas in a bounded container Ω is given by

$$(G) \quad \begin{cases} \theta_t - \Delta \theta = \delta e^\theta + \frac{\gamma-1}{\gamma} \frac{1}{\text{vol } \Omega} \int_{\Omega} \theta_t d\Omega \\ \theta(x,0) = \theta_0(x), \quad x \in \Omega \\ \theta(x,t) = 0, \quad (x,t) \in \partial\Omega \times (0,\infty) \end{cases} \quad .$$

The solution $\theta(x,t)$ of (G) is dominated by the solution $u(x,t)$ of

$$(E) \quad u_t - \Delta u = \delta e^u + \frac{\gamma-1}{\text{vol } \Omega} \delta \int_{\Omega} e^u d\Omega$$

on their common interval of existence. In this paper an extensive analysis (including

existence and invariance results) is given for a class of nonlinear functional equations of the form

$$(F) \quad Lu = f(x, t, u, \Phi u)$$

where L is uniformly parabolic and Φ is a smooth operator which includes (E) as a special case. The analysis is based on the concept of upper and lower solutions for parabolic functional equations.

L. Poland and D. R. Kassoy, "The induction period of a thermal explosion in a gas between infinite parallel plates", *Combustion and Flame* 50, 259-274 (1983).

A study is made of the initiation of gas dynamical processes during the induction period of a high activation energy supercritical thermal explosion in a reactive gas confined between two infinite parallel plates. Solutions are assumed to vary spatially only in the direction perpendicular to the plates. The detailed development of the density, velocity, temperature, and fuel mass fraction fields during the induction period is separated into three phases. During the first phase, occurring on the acoustic timescale of the vessel, conduction-dominated boundary layers generate an acoustic field in a non-dissipative interior core region. The second phase, occurring on the conduction timescale of the vessel, is characterized by a pointwise competition between reaction-generated heat release, conduction, and compression. The Frank-Kamenetskii criteria dividing super- and subcritical systems is found to be the same as that for rigid explosive materials. In a supercritical system, $\delta > \delta_{crit}$, the third phase, of extremely limited duration, is dominated by the development of a tiny self-focusing hot spot embedded within a nearly invariant conduction-dominated field filling most of the vessel. The rapid gas expansion in the hot spot is the source of further, more dramatic gas dynamical processes. The thermal runaway time for the gas system is found to be reduced by

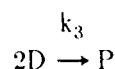
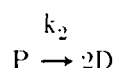
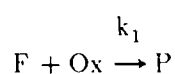
about 25% from that for an analogous rigid explosive over a wide range of values of the Frank-Kamenetskii parameter δ .

This study is unique because the gas-dynamic response to chemical heat addition in a thermal explosion is considered for the first time. Two specific effects are noted. First, we describe the very weak acoustic waves generated during the acoustic period. Although of no significance to the chemistry, these disturbances are responsible for the basically homogeneous pressure rise observed on the conduction scale. Secondly, we examine the velocity field evolving during the induction period to find that the coupling with heat addition leads to a singularity at a specific location. The rapidly growing velocity associated with the singularity produces an accelerating piston-like motion which will generate new and stronger gas-dynamics effects.

The analysis, based on rational perturbation methods, provides insights into the physical phenomena occurring during the induction phase of a thermal explosion. In particular we have demonstrated mathematically that localized heat addition is the source of a rapid gas expansion process within a well defined boundary. That boundary is, in effect, a contact surface separating hot, burned gases from relatively cold fresh mixture. In this sense the localized thermal hot spot is like the reaction center considered by Meyer and Oppenheim [AIAA J. **10**, 1509-1513 (1972)]. This study then sets the stage for an examination of subsequent more rapid processes in which gas expansion will lead to the formation of shock waves and further combustion initiation in the region beyond the original hot spot.

M. A. Birkan and D. R. Kassoy, "The homogeneous thermal explosion with dissociation and recombination", Comb. Sci. Tech. **33**, 135-166, 1983.

Traditional thermal explosion theory is based on the elementary global reaction $F + \text{Ox} \rightarrow P$. As a result, the final temperature in an insulated system is the adiabatic flame value. The latter is too high for real systems where dissociation processes occur at sufficiently large temperature. In order to account for high temperature chemistry we considered the time-history of an adiabatic, spatially homogeneous model of a thermal explosion with the kinetic steps



The first two are considered to be high activation energy reactions while the recombination process has zero activation energy. Kinetic parameters in this model problem are chosen so that dissociation plays a role even early in the process. As a result, the thermal explosion time is affected by the chemical parameters of all the steps. The maximum temperature is reduced from the adiabatic explosion value by the endothermicity of the dissociation process. Relative to the induction time, a long period elapses before the system reaches an equilibrium state where all the products are dissociated. The final temperature is considerably lower than the maximum value because of thermal energy removal by the dissociation process. Other choices of kinetic parameters will lead to a less fully dissociated final state.

This study demonstrated for the first time that kinetic systems with varying levels of activation energy can be treated by asymptotic methods. It provides a framework

which can be used to consider much more complex reaction processes with many species and kinetic steps.

J. F. Clarke, "Combustion in plane steady compressible flow: general considerations and gas dynamical adjustment regions", *J. Fluid Mech.* 136, 139-166 (1983).

By specializing to the case of unit Lewis number and Prandtl number equal to $\frac{3}{4}$, a number of general results for the structure of a plane steady compressible flow field, within which chemical energy is being liberated by a simple Arrhenius type of combustion reaction, can be acquired by the use of elementary arguments. The field is of the semi-infinite variety, with a 'flameholder' presumed to exist at the origin of coordinates. In these circumstances it is necessary to specify the velocity gradient at the inlet to the system or, equivalently, the pressure difference across the field. These quantities cannot be selected arbitrarily, and the nature and extent of the restrictions upon them is fully explored. Since the Mach number of the stream is hypothesized to be a quantity of order unity, local Damköhler numbers are always small. Therefore the field is shown to consist of relatively long regions within which the combustion activity takes place, with embedded thin domains of rapid, almost chemically inert, gasdynamical adjustment, whose dimension is typically that of the conventional shock wave. When the inlet Mach number is less than unity the gasdynamical adjustment domains are always adjacent to the origin, and this is also true under most supersonic inlet conditions.

However, there are some special circumstances for which the shock is detached from the flameholder and is established in the middle of the combustion activity. A specific example is provided by a shock within the induction domain.

These special circumstances are shown to be ultrasensitive to pressure difference across the whole domain. It is also shown that wholly supersonic combustion does exist,

but only under similar conditions of extreme sensitivity to pressure difference.

The general arguments are supported and illuminated by asymptotic analysis based on the large activation energy of the Arrhenius reaction. Space precludes a full asymptotic treatment of the combustion activity but a companion paper that analyses these parts of the general field is authored by Kassoy and Clarke [J. Fluid Mech. 150, 253-280, 1985]. Analysis of the shock within the induction domain, together with results from the case of subsonic inlet Mach numbers, shows that gasdynamical effects can prevent ignition by channelling combustion energy into kinetic energy of the flow at the expense of thermal energy.

A. M. Radhwan and D. R. Kassoy, "The response of a confined gas to a thermal disturbance: rapid boundary heating", J. Engineering Math., 18, 133-156, (1984).

An inert compressible gas confined between infinite parallel planar walls is subjected to significant heat addition at the boundaries. The wall temperature is increased during an interval which is scaled by the acoustic time of the container, defined as the passage time of an acoustic wave across the slab. On this timescale, heat transfer to the gas occurs in thin conductive boundary layers adjacent to the walls. Temperature increases in these layers cause the gas to expand such that a finite velocity exists at the boundary-layer edge. This mechanical effect, which is like a time-varying piston motion, induces a planar linear acoustic field in the basically adiabatic core of the slab. A spatially homogeneous pressure rise and a bulk velocity field evolve in the core as the result of repeated passage of weak compression waves through the gas. Eventually the thickness of the conduction boundary layers is a significant fraction of the slab width. This occurs on the condition timescale of the slab which is typically a factor of 10^6 larger than the acoustic time. The further evolution of the thermomechanical response

of the gas is dominated by a conductive-convective balance throughout the slab. The evolving spatially-dependent temperature distribution is affected by the homogeneous pressure rise (compressive heating) and by the deformation process occurring in the confined gas. Superimposed on this relatively slowly-varying conduction-dominated field is an acoustic field which is the descendent of that generated on the shorter timescale. The short-time-scale acoustic waves are distorted as they propagate through a slowly-varying inhomogeneous gas in a finite space.

This problem is an extension of earlier work [Kasoy, SIAM J. Appl. Math. **36**, 624-634, (1979)] to determine the thermomechanical response of a gas when the temperature rise time is $O(10^{-3} \text{ s.})$. During this period, the boundary heat flux is $O(10^4 \text{ W/m}^2)$. The acoustic noise generated by this disturbance has an intensity of more than 10^2 decibels. A combination of matched asymptotic expansion methods and multiple scale methods are employed to develop solutions involving two length scales and two time scales. In mathematical terms we describe concurrent parabolic and hyperbolic processes. Perhaps of most interest, the analysis of heat transfer on the conduction timescale, $O(10^2 \text{ s.})$ involves acoustic transmission in a slowly varying, spatially dependent background field controlled by conduction. In this finite problem the acoustic field is Fourier-decomposed in order to separate acoustic time dependence from that associated with changes on the longer conduction scale. A variant of the WKB-method is employed to show that the amplitude of each mode grows when the background temperature at a point increases with time. This condition is met when wall heating (as opposed to cooling) occurs on the acoustic timescale. Although a considerable effort has been made in the combustion literature [Oran and Gardner, NRL Memorandum Report 5554, Naval Research Laboratory, 1985] to consider the interaction between travelling

acoustic waves and varying background temperature fields, the present result for standing waves appears to be unique.

This study was motivated by a need to understand the role of acoustic waves generated by a thermal transient in a gas. The mathematical methods and concepts developed in the course of analysis are applicable directly to flame and detonation wave initiation resulting from rapid deposition of energy at a boundary.

J. F. Clarke, D. R. Kassoy and N. Riley, "Shocks generated in a c} under Cnfin ed gas due to rapid heat addition at the boundary. I. Weak shock waves", Proc. R. Soc. London A 393, 309-329, (1984) and "II. Strong shock waves", Proc. R. Soc. London A 393, 331-351, (1984).

Detonation wave initiation occurs when a sufficient amount of energy and power density are deposited into a volume of gas [Lee, Ann. Revs. Phys. Chem. 28, 75-104, 1977]. The sufficiency requirement is almost certainly associated with shock wave generation resulting from the thermomechanical response of a compressible gas to power deposition. In order to study this process in its most elementary form we examined the birth and evolution of a planar shock in a gas confined between parallel walls. Heat flux at the boundary rises from zero to a prescribed value over a timescale shorter than the container acoustic time (say, $O(10^{-3}$ s.)) but at least as large as the time between molecular collisions (say, 10^{-10} s.). In the case of heating times longer than the collision time, weak shocks are generated.

Conductive heating of a thin layer of gas adjacent to the wall induces a gas motion arising from thermal expansion. The small local Mach number at the layer edge has the effect of a piston on the gas beyond. A linear acoustic wave field is then generated in a thicker layer adjacent to the walls. Eventually nonlinear accumulation effects occur on a timescale that is longer than the initial heating time but short com-

pared with t_a' . A weak shock then appears at some well defined distance from the boundary. If the heating rate at the wall is maintained over the longer timescale, then a high temperature zone of conductively heated expanding gas develops. The low Mach number edge speed of this layer acts like a contact surface in a shock tube and supports the evolution of the weak shock propagating further from the boundary. One-dimensional, unsteady solutions to the complete Navier-Stokes equations for an inert gas are obtained by using perturbation methods based on the asymptotic limit $t_a'/t_c' \rightarrow 0$, where t_c' , the conduction time of the region, is the ratio of the square of the wall spacing to the thermal diffusivity in the initial state. The shock strength is shown to be related directly to the duration of the initial boundary heating.

When the heating time is a few multiples of the collision time one finds that the shock is born in the gas layer directly adjacent to the boundary. That layer is initially only a few mean free paths thick. The complete unsteady Navier-Stokes equations are used to describe the evolution of the fully structured shock wave. Of course, the validity of continuum equations for such fast and small scale processes must be tested here in the same sense as that in the steady structure analysis of Gilbarg and Paolucci, *J. Rat. Mech. Anal.* **2**, 617-642, (1953).

Numerical solutions show how a spatial pressure variation is generated adjacent to the boundary, which then evolves into an almost steady shock wave. At a given propagation Mach number this shock generates pressure and temperature changes almost identical to those obtained from Rankine-Hugoniot theory. This consideration verifies the initial value calculation based on the Navier-Stokes equation. If heat addition is continued, a thicker high-temperature expanding layer develops in which the pressure remains uniform. This expanding layer acts like a piston, or a contact surface, the

speed of which is calculated to leading order. In this way the present theory provides a rational basis for the *ad hoc* piston analogies used by earlier authors. In particular it shows the importance of power as a crucial factor in the determination of shock strength.

The mathematical model employed in these papers describes the most fundamental physical processes leading to shock formation. In the course of study, a formal derivation of the Zeldovitch thermal wave equation [Zeldovitch and Raizer, "Physics of shock waves and high temperature hydrodynamic phenomena", Academic Press, (1967)] is given for the first time. The rigorous, constructive analysis, based on asymptotic methods, permitted us to show formally that planar shock wave strength is directly associated with power density in the heated layers. This verifies the results of experimental studies of detonation wave initiation.

J. Bebernes and W. Fulks, "The small heat-loss problem", J. Differential Equations 56, (1985), 324-332.

When the ignition model for a rigid explosive in a bounded container Ω is analyzed by considering the boundary layer effects, one encounters the small heat loss problem:

$$(S) \quad \begin{cases} u_t - u_{xx} = e^u, & x > 0, \quad 0 < t < T \\ u(x, 0) = 0, & x > 0 \\ u(x, t) = 0, & 0 \leq t \leq T. \end{cases}$$

The adiabatic core solution has the form $a(x, t) = -\ln(1-t)$ and for matching one would hope that the solution $u(x, t)$ of (S) uniformly approaches $a(x, t)$ as $x \rightarrow \infty$ and $0 \leq t \leq T < 1$. In this paper, we prove that (S) has a unique solution on $[0, \infty) \times [0, T)$, $T \leq 1$, and that this solution satisfies the asymptotic condition

$\lim_{x \rightarrow \infty} u(x,t) = -\ln(1-t)$, $t \in (0,1)$ and that $u_x > 0$, and $u_t \geq 0$.

This result confirms the predictions made by Kassoy-Poland [SIAM J. Appl. Math. **39**, (1981), 412-430]. It represents a pioneering contribution to an exciting area of current research in which one attempts to describe the shape of the temperature profile as blow-up is approached.

D. R. Kassoy, "Mathematical modeling for planar, steady subsonic combustion waves", Ann. Rev. Fluid. Mech. **17** (1985), 267-287.

A review is given of the theoretical foundations for planar flame and higher speed deflagration modeling when the elementary reaction $A \rightarrow B$ is considered. A unified formulation is constructed for the structure of the reactive flow process downstream of a well-defined origin from which a premixed reactive gas is emanating. Traditional burner-attached low speed flame theory is derived from a high activation energy analysis of the small Mach number flow equations. The special limit of the separated flame (vanishingly small conduction heat transfer to the burner) is derived. The solution is identical to that for the doubly-infinite flame model in which a pseudo-equilibrium state exists far upstream of the reaction zone. It is shown that the classical flame structure is separated from the burner by a much thicker zone in which there is a balance of weak reaction and convection. In the formal sense, this result shows in unique manner that the doubly-infinite flame solution describes only a limited region of the reaction zone downstream of the burner.

Larger burner mass flow rates lead to deflagration solutions in which diffusion and conduction are suppressed relative to convective and reactive effects. This change in the physical control mechanism develops as length scales increase and molecular transport becomes increasingly ineffective. For sufficiently large flow field Mach numbers,

the reaction zone structure is free of transport effects and compressibility plays an increasingly important role. These reactive compressible flows with distributed chemical heat addition have properties associated with convecting thermal explosions. The reaction rate in a material particle of reactive gas accelerates slowly at first. Close to a critical position a very rapid heat release occurs and significant temperature rise takes place. Compressibility effects act to augment or diminish the temperature depending upon the local flow Mach number. The stability properties of these reaction zones, as much as meters in extent for the reaction $A \rightarrow B$, are unknown.

J. Bebernes and A. Bressan, "Global *a priori* estimates for the solution of the initial boundary value problem for a viscous reactive gas", Proceedings Royal Soc. Edinburgh, 80A (1985).

In this paper, we derived a set of global *a priori* estimates on the solution of the complete system of equations governing a heat-conductive, viscous reactive perfect gas confined between two infinite parallel plates. The model as developed by Kassoy-Poland, [Combustion and Flame, 59 (1983), 259-274] and written in Lagrangian coordinates has the form:

$$(L) \quad \begin{aligned} \rho_t + \rho^2 v_x &= 0 \\ v_t &= \lambda_1(\rho v_x)_x - k(\rho\theta)_x \\ \theta_t &= \lambda_2(\rho\theta_x)_x + \lambda_1\rho v_x^2 - k\rho\theta v_x + \delta f(\rho, \theta, z) \\ z_t &= \lambda_3(\rho^2 z_x)_x - f(\rho, \theta, z) \end{aligned}$$

with initial boundary conditions

$$v(0, t) = v(1, t) = z_x(0, t) = z_x(1, t) = 0$$

$$\theta_x(0, t) = \theta_x(1, t) = 0, \quad t > 0$$

and

$$\rho(x,0) = \rho_0(x), \quad v(x,0) = v_0(x), \quad \theta(x,0) = \theta_0(x), \quad z(x,0) = z_0(x).$$

The function $f(\rho, \theta, z) = \epsilon k \rho^{m-1} z^m e^{\frac{\theta-1}{\epsilon \theta}}$ describes the rate of the chemical reaction. The product δf represents the generation of heat by the chemical reaction. The presence of the f -term and the addition of chemical species equation make this one-dimensional problem considerably more complex and interesting than the analogous inert problem.

The Soviet school of combustion theorists — Kazhikov and Shelukin, in particular — have considered the model for a viscous heat-conducting perfect gas bounded by two infinite plates with thermally insulated boundaries but did not allow for heat to be generated by chemical reactions.

With the global *a priori* estimates, local existence theorems can be invoked to establish the global existence of both weak and classical solutions for the one-dimensional problem (L). In particular, we can conclude that no shocks (discontinuous solutions) can develop at any future time.

D. R. Kassoy and J. E. Clarke, "The structure of a steady high-speed deflagration with a finite origin", *J. Fluid Mech.* **150**, 253-280, 1985.

A mathematical model has been developed for a one-dimensional steady high-speed deflagration when a unimolecular decomposition reaction of the Arrhenius type determines the rate of heat addition. The flow evolves from a non-equilibrium origin which represents the exit of an experimental apparatus. This burner configuration permits one to work with a well-posed mathematical system when the kinetics are described in terms of the ordinary Arrhenius rate law. The reactive compressible flow is studied for arbitrary values of the Lewis and Prandtl numbers, for general variations of viscosity, conductivity and diffusivity and for a temperature-dependent specific heat C_p . A complete solution is obtained in the limit of high activation energy when the shortest

possible characteristic reaction time is large with respect to the typical time interval between molecular collisions.

Reaction initiation occurs adjacent to the origin in a region scaled in extent by a modest multiple of the mean free path of the gas. A balance of weak chemical heat-addition and transport effects produces exponentially small, but finite, gradients which can adjust to a wide range of input Mach numbers M . In a subsequent region there is a fundamental balance of convection, reaction and compressibility which leads to a thermal explosion-like ignition process at the dimensional location

$$x_1 = \frac{\epsilon(1-M^2)}{(1-\gamma M^2)h} [u_1 B^{-1} e^{1/\epsilon}]$$

when $M^2 < \gamma^{-1}$ or $M^2 > 1$. Here ϵ is the inverse activation energy parameter, h is the nondimensional heat addition and B is the pre-exponential factor in the Arrhenius rate law. When $M^2 < \gamma^{-1}$ the result is identical with that found by Erpenbeck [Proc. 9th Symp. (Int'l) on Combustion, 442 The Combustion Institute (1963)] in a study of a subsonic reaction zone downstream of a shock. The term in square brackets represents the distance travelled by a fluid particle moving at the initial speed u_1 during the characteristic initial-reaction time $B^{-1} e^{1/\epsilon}$.

As $x \rightarrow x_1$ — a more violent reaction process occurs on a lengthscale short compared with x_1 . Unlike the previous induction zone, where $O(\epsilon)$ changes in reactant concentration and temperature occur, there are $O(1)$ changes in each of the physical variables. The rapid-combustion process, determined by a balance of convection, reaction and compressibility, proceeds until the reactant has nearly vanished. Variations in the temperature and speed with distance are determined by the strong interaction between heat addition and compressibility. The latter effect tends to limit the tem-

perature rise in the subsonic case because thermal energy is readily converted to kinetic energy. Since transport properties are of negligible importance in this zone, the basic conservation equations for mass and momentum and the state equation reduce formally to those which describe the variations from one state of local mechanical and thermal equilibrium to another in a one-dimensional compressible flow with heat addition. However, the energy and reactant-species conservation equations contain Arrhenius kinetic laws which determine the nature of the distributed heat release in the rapid-combustion zone. Thus local states of *chemical* equilibrium (zero reaction rates) do not exist.

The solutions imply that subsonic deflagrations will develop downstream of the initial point for a wide range of downstream pressures, each of which corresponds to exponentially small initial strain rate and temperature gradient. In contrast, a purely supersonic deflagration can exist for a range of downstream pressures only if the initial gradients take on a set of very specific values. Such a process would be unlikely in practice because the gradient control would be impossible.

The high-speed deflagration described here is generally equivalent to the reaction behind a planar shock in the idealized detonation-wave model. It is well known that the interaction between the shock wave and exothermic processes in the reaction zone lead to a basic flow instability which destroys the one-dimensionality of an initially planar wave.

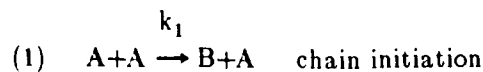
When the input Mach number M in the burner model is sufficiently large, the flame behaves like a convecting thermal explosion. Gradients at the burner are exponentially small with respect to the high-activation-energy parameter limit. The have only the most negligible effect on the global properties of the flame. However, the finiteness of the gradients permits the system to adjust to a wide range of M -values.

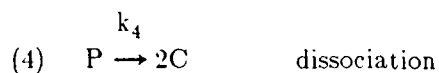
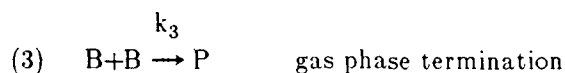
Finally, it should be mentioned that the reaction model employed in the analysis provided the least complex equation system with distributed heat release. An extension of the study to include bimolecular initiation reactions, a model of chain branching, a termination reaction and an equilibrium dissociation-recombination step is desirable, although algebraically complicated.

Related material is contained in D. R. Kassoy and J. F. Clarke, "The high speed deflagration with compressibility effects", in Dynamics of Shock Waves, Explosions and Detonations, Prog. in Astro- and Aeronautics. Eds. J. R. Bowen, A. K. Oppenheim and R. I. Soloukhin, 94 (1984), 175-185.

M. A. Birkan and D. R. Kassoy, "The unified theory for chain branching thermal explosions with dissociation-recombination and confinement effects", Comb. Sci. Tech. 41, 1985, 223-256.

Traditional models of chain branching reactions describe radical generation in an isothermal process [Strehlow, Fundamentals of Combustion, Krieger, 1979]. Only recently Kapila [J. Eng. Math. 12 (1978), 221] developed a more inclusive model which includes the evolution of a thermal explosion resulting from radical recombination. The chain branching thermal explosion process provides a fertile ground for developing mathematical methods capable of describing complex, thermally active reaction events. High activation energy asymptotic methods are used to describe the time-history of a spatially homogeneous, constant volume process governed by the following generic kinetic steps:





The chain initiation step is an endothermic low temperature reaction with a very high activation energy. The chain branching reaction has a large but smaller activation energy and is also endothermic. Large heat release is characteristic of the termination step which occurs with zero activation energy. The dissociation-recombination processes occur at high temperatures and control the final equilibrium state. In the analysis, kinetic parameters are chosen to ensure that the final state is only partially dissociated.

High activation energy asymptotics are used to describe this 5-step, 4-reactant process. The analysis demonstrates quite succinctly that asymptote methods can be employed profitably for a complex reaction scheme. Given patience and algebraic reliability, it appears likely that kinetic schemes of considerably greater complexity can be handled with asymptotic formulations. It is to be stressed that many of the subproblems, representing specialized distinguished limits of the full equation system, are highly nonlinear and require numerical solutions. These calculations are, however, more elementary than numerical computations for the full equations because the asymptotic analysis has permitted one to determine the magnitudes of the dependent variables in each of the scaled time regimes.

The initiation reaction (1) generates tiny amounts of radical B at first. Over a long period the propagation reaction (2) produces increasing numbers of B along with some temperature rise associated with weak termination. Eventually, a rapid increase in B occurs as a critical time is approached. This chain explosion generates a significant radical population. Recombination then becomes more important from the energetic viewpoint and the system temperature rises rapidly. The resulting thermal explosion accelerates the rates of (1) and (2) so that rapid depletion of A occurs. The maximum temperature is larger than the adiabatic value because finite volume compression has been incorporated in the model. The subsequent dissociation process gradually lowers the temperature. There follows a very long approach to equilibrium as recombination of dissociated fragments takes place. The results for the generic kinetic model in (1)-(5) are used with kinetic data from $\text{H}_2\text{--O}_2$ reactions to show that dimensional timescales for individual reaction processes (initiation, propagation, chain branching, dissociation and recombination) are physically reasonable. The success of this study should motivate further efforts to use asymptotic methods for real kinetic schemes.

J. Bebernes, D. Eberly, and W. Fulks, "Solution profiles for some simple combustion models", *Nonlinear Analysis: Theory, Methods and Applications*, **8** (1985),

Using phase space techniques, the solution shapes for the Gelfand problem $-\Delta u = \delta e^u$ and the perturbed Gelfand problem $-\Delta u = \delta \exp(\frac{u}{1+\epsilon u})$, $\delta > 0$, $\epsilon > 0$ are analyzed. Both of these models play a fundamental role in the mathematical theory of thermal explosions for finite rigid and gaseous systems. For rigid systems the physical processes are determined by a pointwise balance between chemical heat addition and heat loss by conduction. During the inductive period, with a duration meas-

ured by the conduction time scale of the bounding container, the heat released by the chemical reaction is redistributed by thermal conduction. As the temperature of the container increases, the reaction rate grows dramatically. Eventually the characteristic time for heat release becomes significantly smaller than the conduction time in a well-defined hot spot embedded in the system. Then the heat released is used almost entirely to increase the hot spot temperature. Both the models studied detect this hot spot development in a very precise manner. For example, for a ball $B_1 \subset \mathbb{R}^3$, the minimal solution of the Gelfand problem is bell-shaped, that is, exhibits the hot spot, for a range of parameter values δ , $\bar{\delta} < \delta < \delta^*$. When $0 < \delta < \bar{\delta}$, the physically significant minimal solution is concave down while all other solutions are bell-shaped. Here δ^* is the Frank-Kamenetskii critical value and $\bar{\delta}$ is a uniquely determined parameter value.

J. Bebernes and D. Kasso, "Solution profiles and thermal runaway", Lectures in Applied Mathematics, 1985, to appear.

This is an expository description of how thermal runaway occurs for the induction period model of a high activation energy thermal explosion in a bounded container. Assuming a slab geometry, the temperature perturbation $\theta(x,t)$ (solution of $(*)$ $\theta_t = \Delta\theta + \delta e^\theta$) blows up at a single point $x = 0$ as $t \rightarrow T$ and $\theta(x,t) \rightarrow \theta_e(x)$ for $0 < x \leq 1$. In principle $\theta_e(x)$ is found from an initial value numerical solution of $(*)$. Assuming $\theta_e(x)$ as a known quantity, a final value theory for this problem is described. This allows one to predict the shape of the temperature $\theta(x,t)$ in a neighborhood of the singularity.

J. Bebernes and W. Troy, "Nonexistence for the Kassoy problem", SIAM J. of Math. Analysis, to appear.

When blow-up or thermal runaway occurs in finite time for the thermal explosion of a nondeformable material, the developing hot spot becomes unbounded at a single point of the container if it is radially symmetric. These supercritical processes which are characterized by the appearance of this singularity at a finite time T have been considered earlier by Kassoy-Poland and Kapila. Using computational methods for symmetric slab, cylindrical, and spherical geometries, they predict that $\theta(x,t)$ becomes unbounded at the symmetry point $x = 0$ at time T . Elsewhere $\theta(x,t) \rightarrow \theta_e(x)$, $x \in \Omega$, $x \neq 0$, as $t \rightarrow T$. By applying a final-value asymptotic analysis at T , they predict the character of the singularity function $\theta_e(x)$. This prediction is based on the existence of a nontrivial solution of $y'' - \frac{x}{2} y' + e^y - 1 = 0$, $y'(0) = 0$, and $y(x) \sim -2 \ln x + c$ as $x \rightarrow \infty$. By using connectedness and shooting technique arguments, we prove that no such solution can exist. This means a more detailed analysis of the blow-up singularity is required and this has been done in subsequent papers.

J. Bebernes, "A description of blow-up for the solid fuel ignition model", Proc. of Equadiff b, Springer-Verlag, 1985, to appear.

In this paper we announce our result concerning the precise description of the asymptotic behavior of the solution $u(x,t)$ of $u_t - \Delta u = e^u$. For a bounded ball B_R in \mathbb{R}^1 or \mathbb{R}^2 (slab or cylinder geometry), the radially symmetric solution $v(r,t)$ of $v_t = v_{rr} + \frac{n-1}{r} v_r + e^v$ with $v(r,0) = \phi(r)$, $r \in [0,R]$ and $v_r(0,t) = 0$, $v(R,t) = 0$ satisfies $v(r,t) - \ln(T-t)^{-1} \rightarrow 0$ uniformly on $0 \leq r \leq c(T-t)^{1/2}$, $c > 0$ as $t \rightarrow T^-$. This shows that the shape of the developing hot spot is flat as the blow-up singularity is approached.

J. Bebernes, "Solid fuel combustion — some mathematical problems", *Rocky Mountain J. Math.*, 1986.

This is an expository paper which surveys and collects together known results for mathematical models of rigid thermal systems.

List of Publications

1982

D. R. Kassoy, "A Note on Asymptotic Methods for Jump Phenomena", *SIAM J. Applied Math.*, **42** (1982), 926-932.

J. Bebernes and A. Bressan, "Thermal behavior for a confined reactive gas", *J. Differential Equations*, **44** (1982), 118-133.

J. Bebernes and R. Ely, "Comparison techniques and the method of lines for a parabolic functional equation", *Rocky Mountain J. Math.*, **12** (1982), 723-733.

J. Bebernes, "Ignition for a gaseous thermal reaction", *Proceedings of Equadiff 5*, Teubner Text, 1982, Band 47, M. Gregus, Editor, 34-36.

J. Bebernes and D. R. Kassoy, "Self-ignition for thermal reactions", *Transactions of the twenty-seventh conference of Army mathematicians*, ARO Report 82-1, 687-706.

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M. A. Birkan and D. R. Kassoy, "The Homogeneous Thermal Explosion with Dissociation and Recombination", *Comb. Sci. and Tech.*, **33** (1983), 125-139.

J. F. Clarke, "Combustion in plane steady compressible flow: General considerations and gas dynamical adjustment regions", *J. Fluid Mech.* **136** (1983), 139-166.

D. R. Kassoy and J. Poland, "The induction period of a thermal explosion in a gas between infinite parallel plates", *Combustion and Flame*, **50** (1983), 259-274.

J. Bebernes and R. Ely, "Existence and invariance for parabolic functional equations, *Nonlinear Analysis: Theory, Methods, and Applications*, **7** (1983), 1225-1236.

1984

D. R. Kassoy and J. F. Clarke, "The high speed deflagration with compressibility

effects", *Dynamics of Shock Waves, Explosions, and Detonations*, Prog. in Astronautics and Aeronautics, eds. J. R. Bowen, N. Manson, A. K. Oppenheim and R. I. Soloukhin, 94 (1984), 175-185.

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J. F. Clarke, D. R. Kassoy and N. Riley, "Shocks generated in a confined gas due to rapid heat addition at the boundary. I. Weak shock waves", *Proc. Roy. Soc. London A393* (1984), 309-329.

J. F. Clarke, D. R. Kassoy and N. Riley, "Shocks generated in a confined gas due to rapid heat addition at the boundary. II. Strong shock waves", *Proc. Roy. Soc. London A393* (1984), 331-351.

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D. R. Kassoy and J. F. Clarke, "The structure of a high speed deflagration with a finite origin", *J. Fluid Mech.*, 150 (1985), 253-280.

M. A. Birkan and D. R. Kassoy, "The unified theory for chain branching thermal explosions with dissociation-recombination and confinement effects", *Comb. Sci. and Technology*, 44, #5 and #6 (1985), 223.

D. R. Kassoy, "Mathematical modelling for planar, steady, subsonic combustion waves", *Annual Reviews of Fluid Mechanics*, 17 (1985), 267-287.

J. Bebernes and W. Fulks, "The small heat-loss problem", *J. Differential Equations*, 56 (1985), 324-332.

J. Bebernes and A. Bressan, "Global *a priori* estimates for the solution of the initial boundary value problem for a viscous reactive gas", *Proceedings Royal Soc. Edinburgh*, 80A (1985),

J. Bebernes, D. Eberly, and W. Fulks, "Solution profiles for some simple combustion models", *J. Nonlinear Analysis: Theory, Methods, and Applications*, 8 (1985),

To Appear

J. Bebernes, "Solid fuel combustion — some mathematical problems", *Rocky Mountain Journal of Mathematics*, to appear.

J. Bebernes and D. Kassoy, "Solution profiles and thermal runaway", *Lectures in Applied Mathematics*,

J. Bebernes, "A description of blow-up for the solid fuel ignition model", *Proceedings of Equadiff 6*, Springer Verlag, 1985, to appear.

J. Bebernes and W. Troy, "Nonexistence for the Kassoy problem", *SIAM J. Math. Analysis*, to appear.

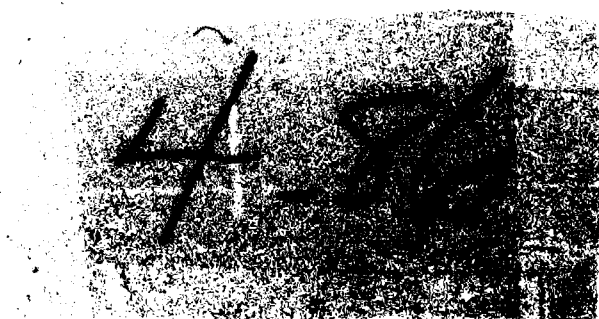
Participating Scientific Personnel

The participating personnel include the principal investigators, their students and several distinguished visiting researchers.

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|--------------|--|
| J. Bebernes | Professor, Mathematics |
| M. Birkan | Ph.D., Mechanical Engineering University of Colorado, August 1984 |
| A. Bressan | Ph.D., Mathematics, August 1982; and Summer visitor, 1985 |
| J. F. Clarke | Visiting Research Associate; and Professor, Aerodynamics, Cranfield Institute of Technology, Cranfield, England |
| D. Eberly | Ph.D., Mathematics, August 1984 |
| D. R. Kassoy | Professor, Mechanical Engineering |
| K. Kirkoppru | Ph.D., in progress |
| A. Radhwan | Ph.D., Mechanical Engineering, 1981 |
| M. Wang | Ph.D., in progress |

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